Exploring the role of model parameters and regularization procedures in the thermodynamics of the PNJL model

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Abstract. The equation of state and the critical behavior around the critical end point are studied in the context of the Polyakov–Nambu–Jona–Lasinio model. We prove that a convenient choice of the model parameters is crucial to get the correct description of isentropic trajectories. The physical relevance of the effects of the regularization procedure is insured by the agreement with general thermodynamic requirements. The results are compared with simple thermodynamic expectations and lattice data.

Keywords: Polyakov-Nambu-Jona-Lasinio model, equation of state, isentropic trajectories

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INTRODUCTION

Understanding the QCD phase diagram in the (T,μ) -plane is of central importance in theoretical and experimental heavy-ion physics. Various results from QCD inspired models indicate that at low temperatures the transition may be first order for large values of the chemical potential; on the contrary a crossover is found for small chemical potential and large temperature. This suggests that the first order transition line may end when the temperature increases, the phase diagram thus exhibiting a (second order) critical endpoint (CEP) that can be detected by a new generation of experiments with relativistic nuclei, as the CBM experiment (FAIR) at GSI. Fodor and Katz [1] claim the values $T^{CEP} = 162$ MeV and $\mu^{CEP} = 360$ MeV for such a critical point, although its precise location is still a matter of debate

As a reliable model that can treat both the chiral and the deconfinement phase transitions, we can consider the Polyakov loop extended Nambu–Jona–Lasinio (PNJL) model [2, 3]. In the PNJL model the deconfinement phase transition is described by the Polyakov loop. This improved field theoretical model is fundamental for interpreting the lattice QCD results and extrapolating into regions not yet accessible to lattice simulations. A non trivial question in NJL type models is the choice of the parameter set and of the regularization procedure. In fact, one should keep in mind that this type of models are used not only to describe physical observables in the vacuum but also to explore the physics at finite temperature and chemical potential. As it is well known, the order of the phase transition on the axis of the (T,μ) -plane is sensitive to the values of the parameters, most notably to the value of the ultraviolet cutoff needed to regularize the integrals. In the pure NJL model a large cutoff leads to a second order transition, a small cutoff to a first order one [4]. An interesting feature to be noticed is that the requirement of global accordance with physical spectrum is obtained with values of the cutoff for which the transition is first order on the T=0 axis and a smooth crossover on the $\mu=0$ axis of the phase diagram. However, it has also been shown that different parameter sets, although providing a reasonable fit of hadronic vacuum observables and predicting a first order phase transition, will lead to different physical scenarios at finite T and μ [5, 6]. For instance, the absolute stability of the vacuum state at T=0 is not always insured.

The consequences of the choice of the parameter set for the scenarios in the (T,μ) -plane have not been discussed in the framework of the PNJL model, where the most popular parameter set does not allow for the absolute stability of the vacuum at T=0. In the present work, our main goal is to analyze this problem and we will assume that the most reliable parametrization of both NJL and PNJL models positively predicts the existence of the CEP in the phase diagram, together with the formation of stable quark droplets in the vacuum state at T=0. Concerning the regularization of some integrals, since, as it has been noticed by several authors, the three dimensional cutoff is only necessary at zero temperature, the dropping of this cutoff at finite T is also carefully analyzed in this work.

MODEL LAGRANGIAN

The generalized Lagrangian of the quark model for $N_f = 2$ light quarks and $N_c = 3$ color degrees of freedom, where the quarks are coupled to a (spatially constant) temporal background gauge field (represented in term of Polyakov loops), is given by [3]:

$$\mathcal{L}_{PNJL} = \bar{q} (i \gamma^{\mu} D_{\mu} - \hat{m}) q + \frac{1}{2} g [(\bar{q} q)^{2} + (\bar{q} i \gamma_{5} \vec{\tau} q)^{2}] - \mathcal{U} (\Phi[A], \bar{\Phi}[A]; T), \tag{1}$$

where the quark fields q = (u,d) are defined in Dirac and color spaces, and $\hat{m} = \text{diag}(m_u, m_d)$ is the current quark mass matrix. The pure NJL sector contains three parameters: the coupling constant g, the cutoff Λ and the current quark mass $m = m_u = m_d$, to be determined by fitting the experimental values of several physical quantities (see Table 1).

The quarks are coupled to the gauge sector *via* the covariant derivative $D^{\mu} = \partial^{\mu} - iA^{\mu}$. The strong coupling constant g_{Strong} has been absorbed in the definition of A^{μ} .

The Polyakov loop Φ (the order parameter of Z_3 symmetric/broken phase transition in pure gauge) is the trace of the Polyakov line defined by: $\Phi = \frac{1}{N_c} \langle \langle \mathscr{P} \exp i \int_0^\beta d\tau A_4 (\vec{x}, \tau) \rangle \rangle_{\beta}$, where $\langle \langle \ldots \rangle \rangle_{\beta}$ with $\beta = 1/T$ is the thermal expectation value in the grand canonical ensemble.

TABLE 1. Set of parameters (Λ, g, m) used in the NJL sector of the PNJL model and the physical quantities chosen to fix the parameters.

	Λ	g	m	$ \langle \bar{\psi}_u \psi_u \rangle ^{1/3}$	f_{π}	m_{π}	M
	[GeV]	$[GeV^{-2}]$	[MeV]	[MeV]	[MeV]	[MeV]	[MeV]
Set A	0.590	7.0	6.0	241.5	92.6	140.2	400
Set B	0.651	5.04	5.5	251	92.3	139.3	335

The pure gauge sector is described by an effective potential $\mathscr{U}(\Phi[A], \bar{\Phi}[A]; T)$ that takes the form

$$\frac{\mathscr{U}(\Phi,\bar{\Phi};T)}{T^4} = -\frac{b_2(T)}{2}\bar{\Phi}\Phi - \frac{b_3}{6}(\Phi^3 + \bar{\Phi}^3) + \frac{b_4}{4}(\bar{\Phi}\Phi)^2, \qquad (2)$$

where

$$b_2(T) = a_0 + a_1 \left(\frac{T_0}{T}\right) + a_2 \left(\frac{T_0}{T}\right)^2 + a_3 \left(\frac{T_0}{T}\right)^3.$$
 (3)

The coefficients a_i and b_i of the Polyakov loop effective potential are chosen (see [3]) to reproduce, at the mean-field level, the results obtained in lattice calculations. The numerical values are: $a_0 = 6.75$, $a_1 = -1.95$, $a_2 = 2.625$, $a_3 = -7.44$, $b_3 = 0.75$ and $b_4 = 7.5$. In addition, we choose $T_0 = 190$ MeV at finite temperature and $T_0 = 270$ MeV at finite temperature and chemical potential.

The important point of our argumentation about the choice of the model parameters comes from the comparison between the point $(0, \mu_c)$ of the phase diagram, where μ_c is the position of the first order line at zero temperature, and the point $(0, M_{vac})$, where $M_{vac} = M$ is the mass of the u, d-quark in the vacuum. Two special cases are observed [5]:

- (i) For set A, the first order phase transition occurs at μ_c such that $\mu_c < M_{vac}$, and consequently the phase transition connects the vacuum state ($\rho_q = 0$) directly with the phase of partially restored chiral symmetry ($\rho_q = \rho_c$). This is compatible with the existence of stable quark matter, indicating the possibility for finite droplets to be in mechanical equilibrium with the vacuum at zero pressure [5, 6].
- (ii) For set B, $\mu_c > M_{vac}$, so the phase transition connects a $\rho_q \neq 0$ phase of massive quarks with the phase of partially restored chiral symmetry ($\rho_q = \rho_c$). From the physical point of view, this scenario is unrealistic because it predicts the existence of a low-density phase of homogeneously distributed constituent quarks [5].

So, although we can choose several sets of parameters which fit physical observables in the vacuum, we notice, however, that the value of the cutoff itself does have some impact on the characteristic of the first order phase transition.

Comparing the two sets of parameters A and B (see Table 1) we verify that for larger values of the cutoff, as in set B, a more strong attraction is necessary both to reproduce the physical values in the vacuum and to insure a first order phase transition. The more realistic choice is provided by set A with important implications on the reliability of isentropic trajectories as we will discuss in the sequel.

Concerning the regularization of some integrals, since the three dimensional cutoff is only necessary at zero temperature, the dropping of this cutoff at finite T is also considered. This procedure allows for the presence of high momentum quark states, leading to interesting physical consequences, as it has been shown in [7], where the advantages and drawbacks of this regularization have been discussed in the context of the NJL model. We will enlarge the use this procedure to the PNJL model and discuss its influence on the behavior of several relevant observables. So, we will consider two different regularization procedures at $T \neq 0$:

- (i) Case I, where the cutoff is used only in the integrals that are divergent ($\Lambda \to \infty$ in the convergent ones).
- (ii) Case II, where the regularization consists in the use of the cutoff Λ in all integrals.

Let us notice that the choice of a regularization procedure is a part of the effective modeling of QCD thermodynamic. Indeed we found that a comprehensive study of the differences between the two regularization procedures (with and without cutoff on the quark momentum states at finite temperature) is necessary to have a better understanding of the PNJL model and the role of high momentum quarks around the phase transition. The physical relevance of our numerical solutions is insured by demanding the agreement with general thermodynamic requirements. In particular, we will verify that the correct description of isentropic lines is closely related with the parameter choice in the pure NJL sector.

NUMERICAL RESULTS AND CONCLUSIONS

To check the usefulness of the regularization procedure we start by considering our numerical results at vanishing quark chemical potential. To this purpose, we plot the scaled pressure and the energy as functions of the temperature in Fig. 1. The transition to the high temperature phase is a rapid crossover rather than a phase transition and, consequently,

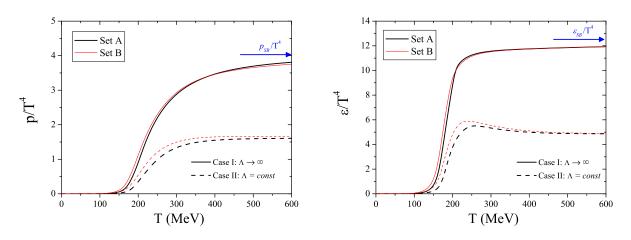


FIGURE 1. Scaled pressure (p) and energy per particle (ε) as a function of the temperature at zero chemical potential for both sets of parameters A and B, and both regularization procedures.

the pressure and the energy densities, which have a similar behavior, are continuous functions of the temperature.

We verify that the inclusion of the Polyakov loop together with the regularization procedure implemented in case I, is essential to obtain the required increase of extensive thermodynamic quantities, insuring the convergence to the Stefan–Boltzmann (SB) limit of QCD. Some comments are in order concerning the role of the regularization procedure for $T > T_c$, where T_c is the reduced temperature. In this temperature range, due to the presence of high momentum quarks, the physical situation is dominated by the significative decrease of the constituent quark masses by the $q\bar{q}$ interactions. This allows for an ideal gas behavior of almost massless quarks with the correct number of degrees of freedom. In this context both sets of parameters provide similar conclusions as can be seen in Figure 1.

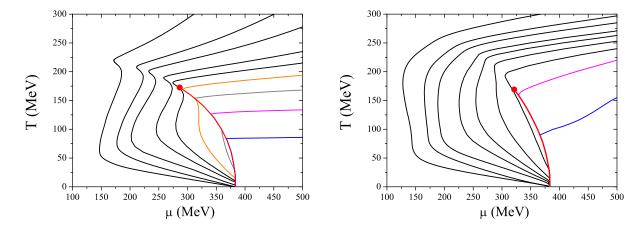


FIGURE 2. Isentropic trajectories in the (T,μ) -plane for case I (left panel) and case II (right panel) using the parameter set A. The following values of the entropy per baryon number have been considered: $s/\rho_q = 1, 2, 3, 4, 5, 6, 8, 10, 15$ (anticlockwise direction).

The advantage of our phenomenological model is the possibility to provide equations of state at nonzero chemical potential too [8]. So, we can also test its ability to reproduce recent progress in lattice QCD with small non vanishing chemical potential.

The isentropic lines play a very important role in the understanding of thermodynamic properties of matter created in relativistic heavy ion collisions. Some model calculations predict that in a region around the CEP the properties of matter are only slowly modified as the collision energy is changed, as a consequence of the attractor character of the CEP [9].

Our numerical results for the isentropic lines in the (T,μ) -plane are shown in Fig. 2, where we have used set A of parameters and both regularization procedures.

We start the discussion by analyzing the behavior of the isentropic lines in the limit $T \to 0$. We point out that, as already referred by other authors [10], in this limit: (i) $s \to 0$, according to the third law of thermodynamics; and (ii) for $s/\rho_q = const$, we have to insure that also $\rho_q \to 0$. However, the satisfaction of the condition (ii) is only provided when $\mu \le M_{vac}$ as discussed above. In spite of the general use of set B in the literature of the PNJL model, only set A satisfies this ansatz. We remember that with set A we are, at T=0, in the presence of droplets (states in mechanical equilibrium with the vacuum state at P=0). Consequently, all isentropic trajectories directly terminate at the first order transition line at T=0. So, for set A it is verified that $s\to 0$ and $\rho_q\to 0$ in the limit $T\to 0$, as it should be.

In conclusion, our convenient choice of the model parameters allows a first order phase transition that is stronger than in other treatments of the NJL (PNJL) model. This choice is crucial to obtain important results: the criterium of stability of the quark droplets [5, 6] is fulfilled, and, in addition, simple thermodynamic expectations in the limit $T \to 0$ are verified.

At $T \neq 0$, in the first order line, the behavior we find is somewhat different from those claimed by other authors [12] where a phenomena of focusing of trajectories towards the CEP is observed. For case I (see Figure 2, left panel) we see that the isentropic lines with $s/\rho_q=1,...,4$ come from the region of symmetry partially restored and attain directly the phase transition, going along with the phase transition as T decreases until it reaches T=0. The same behavior is found for case II when $s/\rho_q=1,2$ (see Figure 2, right panel). For case II, we also observe, in a small range of s/ρ_q around 3, a tendency to convergence of these isentropic lines towards the CEP. These lines come from the region of symmetry partially restored in the direction of the crossover line. For smaller values of s/ρ_q , the isentropic lines turn about the CEP and then attain the first order transition line. For larger values of s/ρ_q the isentropic trajectories approach the CEP by the region where the chiral symmetry is still broken, and also attain the first order transition line after bending toward the critical point. As already pointed out in [10], this is a natural result in these type of quark models with no change in the number of degrees of freedom of the system in the two phases. As the temperature decreases a first order phase transition occurs, the latent heat increases and the formation of the mixed phase is thermodynamically favored.

In the crossover region, for both cases, the behavior of the isentropic lines is qualitatively similar to the one obtained

in lattice calculations [11] or in some models [12]. On the other hand, the isentropic trajectories in the phase diagram indicate that the slope of the trajectories goes to large values for large T.

Summarizing, we have considered the PNJL model as one of the prototype models of dynamical symmetry breaking of QCD and investigated the phase structure at finite T and μ . Working out of the chiral limit, a CEP which separates the first and the crossover line is found. Two important points of our model calculation concern the choice of the model parameters with the emphasis on the parameter choice which is compatible with the formation of stable droplets at zero temperature. The effects of two regularization procedures at finite temperature, one that allows high momentum quark states to be present (case I) and the other not (case II), have also been discussed. We conclude that the choice of the model parameters has important consequences in order to obtain the correct asymptotic low temperature behavior. In the zero temperature limit, the chemical potential approaches a finite value that must satisfy to the condition $\mu_c < M_{vac}$. Only the set of parameters A insures this condition that allows us to obtain both s = 0 and $\rho_q = 0$. In addition, the regularization procedure is important for obtaining agreement with the asymptotic behavior above T_c .

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